

Special Issue

Theoretical Investigations on Nanomaterials

Message from the Guest Editor

A bulk solid contains only a small concentration of surface atoms; as a result, broken chemical bonds on the exterior contribute minimally to material properties. For a particle, the surface-to-volume ratio scales inversely with linear dimensions and the role of the surface increases, eventually becoming dominant when the particle reduces to nanoscale, leading to the particle properties being drastically different from those of the bulk. Theoretical investigations and simulations are being recognized as one of the complementary approaches to experiments investigating the physical origin of the outstanding properties of nanomaterials and to predict the properties of newly designed ones. The continuous development of computational hardware and algorithms and the emerging of new simulation technologies, also enable people to use more realistic models for the investigation of the properties of nanomaterials in situ. We welcome submissions of research and review articles on advances in the field of theoretical investigations and simulations regarding nanomaterials.

Guest Editor

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Deadline for manuscript submissions

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Message from the Editor-in-Chief

Nanoscience and nanotechnology are exciting fields of research and development, with wide applications to electronic, optical, and magnetic devices, biology, medicine, energy, and defense. At the heart of these fields are the synthesis, characterization, modeling, and applications of new materials with lower nanometer-scale dimensions, which we call “nanomaterials”. These materials can exhibit unusual mesoscopic properties and include nanoparticles, coatings and thin films, metal–organic frameworks, membranes, nano-alloys, quantum dots, self-assemblies, 2D materials such as graphene, and nanotubes. Our journal, *Nanomaterials*, has the goal of publishing the highest quality papers on all aspects of nanomaterial science to an interdisciplinary scientific audience. All of our articles are published with rigorous refereeing and open access.

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